**2nd quantization**

Guess we’ll try out a few bases…

**Some operators in position basis**

ψ(x), ψ†(x) are annihilation/creation operators in position space. Let’s look at the density operator first. We have:



and so,



Let’s consider total spin :



where **S**σσ´ = (ℏ/2)[σx**i** + σy**j** + σz**k**] and σσ´ are indices and σx,y,z are the Pauli-spin matrices. From this we can see the spin-densiity would just be:



We can specialize. Recall,



So,



Can do a couple more,



This kind of makes sense, as application of this operator would destroy a spin-down, and then create a spin-up. So it raises the spin basically. And,



This also makes physical sense. The polarization operator is:



And now let’s consider the current density.



The usual way to work this out would be….leaving spin out for the moment:



And now we have:



So filling this in,



We could write this as:



with the understanding that ReA means (1/2)(A + A†). And let’s try another way:



Which is correct. And one more way….we’ll first define the total current (leaving spin out again):



And then switch bases:



I think the overall gradient terms can be neglected as they would introduce surface terms at infinity. And one would suppose that the occupation numbers at infinity are zero? In that case we’d have:



At this point we would identify the current density as:



If we include spin, then we’ll get:



We’ll of course recognize the close similarity this has with the current of a single particle wavefunction. There is a nice identity relating the time derivative of the polarization operator to the current operator:



Then we note that the gradient of **r** is just the unit tensor – its easy to see in Cartesian coordinates. So we have,



This holds for particles w and w/o spin. This formula we used in the electrodynamics folder. Of course, the time derivative of the polarization operator can be calculated without an explicit formula for P(x,t) by simply commuting it with the governing Hamiltonian. Similar procedures can be used to define a heat current, energy current, etc. Let’s do momentum, unfortunately also designated **P**(t).



So,



An expression for the kinetic energy – this time including spin from beginning:



So we have:



with implicit summation over spin indices. Let’s do a one particle potential. We’d have:



Correspondingly, a one particle potential would be represented in the position basis as



If the interaction is spin-independent, then this would reduce to:



A two-particle potential would be represented as follows.



So in the worst-case scenario, where the interaction is spin-dependent, we’d get:



where we’ve used the even-ness of the potential. If the interaction is spin-independent, then we can see that V2σσ´σ´´σ´´´(x-x´) → V2(x-x´)δσ´σ´´δσσ´´´. And so we have:



Let’s do the spin operator,



So we could say the spin density operator is:



Recall from QM Time-Independent folder that (ℏ set to 1),



So filling this in,



Now consider a 2nd quantized spin-orbit interaction:



So,



**Time development in position space**

Let’s consider a general time-independent H in position space. Let’s allow a spin-dependent single particle potential (like say if we had an external magnetic field), but presume a spin-independent interaction:



Then the equation of motion of the annihilation operator would be:



Working it out a little more,



and,



which is,



where



is the density operator. Note the similarity to the time dependent Schrödinger equation in position space. If V1 is spin-independent, then the equation will be diagonal in spin indices.

**Translation Operator**

So I’d like to consider what happens when we operate on the creation/annihilation operators with various symmetry operators. So I’ll do the translation operator first,



So operating on it, we have:



where the last line is using the Baker-Hausdorf formula (see Foundations/Continuous Symmetries). So we have to evaluate that commutator,



So we can see that:



Taking the dagger of both sides, we have:



A faster way to do this would be, recalling the properties of the translation operator in the Foundations/Parity file:



And taking the dagger of both sides gives us the other result. So altogether we have:



**Example**

Consider the free particle Hamiltonian. Let’s verify that it’s translationally invariant,



So it is, as we expect.

**Spin-Rotation Operator**

Let’s say we did a 180o spin-rotation about the y-axis. Then using the rotation operator D(π**j**) = e-iπS\_y), and recalling from the QM Foundations/Rotation file that:

D(π**j**)|σ> = -sgn(σ)|σ>, we have:



Or could’ve said,



Either way, multiplying both sides by D†(α)….D(α), we get:



Just to make sure this is correct, let’s construct the total spin rotation operator. This should probably be:



If we just consider a π rotation about the y axis, then we have:



And we’d like to know what we have for, D†(π)ψσ(x)D(π). Let’s consider the general rotation operator about the y-axis:



Then we have:



Hopefully we can solve the differential equation. Well go back to the penultimate line,



So we have a linear coupled differential equation. Shouldn’t be too bad. Could put in terms of eigenvectors/values. But maybe easier to write out explicitly:



which is:



Taking derivative of the second and plugging into the first, we have:



where A and B are arbitrary operators to be solved for. And then the other guy would be:



Initial conditions are that: ψ↓(α=0)(r) = ψ↓(r), and ψ↑(α=0)(r) = ψ↑(r). So,



So the solution is:



And we finally have:



We might write this as:



Could write this together as:



And we note that this matrix is in fact the representation of D(1/2)(α) in the spinor basis (see Foundations/Rotation file). Well when we plug in α = π, we get exactly what we found before,



Might as well continue and do the other two rotations too. So consider an x-rotation:



Then we have:



Writing out explicitly,



which is:



Taking derivative of the second and plugging into the first, we have:



where A and B are arbitrary operators to be solved for. And then the other guy would be:



Initial conditions are that: ψ↓(α=0)(r) = ψ↓(r), and ψ↑(α=0)(r) = ψ↑(r). So,



So the solution is:



And we finally have:



We might write this as:



Could write this together as:



Again, we note that this matrix is in fact the representation of D(1/2)(α) in the spinor basis (see Foundations/Rotation file). Well when we plug in α = π, we get:



Could do the z-rotation guy, but whatever.

**Parity Operator**

Now let’s look at the parity operator.



and taking the dagger of both sides, we have altogether,



**Time-Reversal Operator**

And now let’s tackle Time-Reversal. Recall it’s not unitary, so Θ-1 ≠ Θ†.



I wonder about that phase factor. Taking dagger of both sides might be kind of problematic. So I’ll just repeat, and this puts the phase factor on surer ground:



Surrounding both sides of our equation with Θ-1….Θ, and recalling Θ is anti-linear, we now see that:



Well it seems this is wrong. Not sure how. Probably same reason the Emperor came back. Online I see that we should instead be saying:

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This could be reconciled with our derivation if we were to go back and say that Θ|0> ≠ |0>, but rather Θ|0> = i|0>. I don’t know the motivation for this, but it isn’t *obviously* wrong, to me. And then we’d end up with:

